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Poly[μ_2-aqua-aqua-μ_5-naphthalene-2,7-disulfonato-strontium]

Shan Gao[a] and Seik Weng Ng[b,c]*

[a]Key Laboratory of Functional Inorganic Material Chemistry, Ministry of Education, Heilongjiang University, Harbin 150080, People's Republic of China, [b]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia, and [c]Chemistry Department, Faculty of Science, King Abdulaziz University, PO Box 80203 Jeddah, Saudi Arabia
Correspondence e-mail: seikweng@um.edu.my

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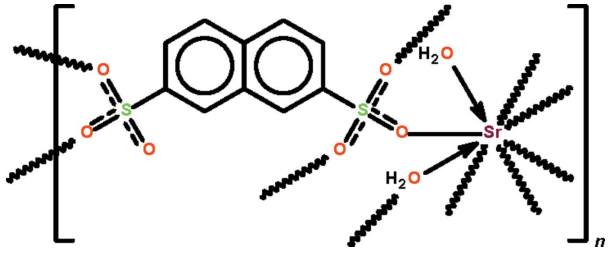
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.028; wR factor = 0.071; data-to-parameter ratio = 15.6.

In the crystal structure of the polymeric title compound, $[Sr(C_{10}H_6O_6S_2)(H_2O)_2]_n$, the naphthalene-2,7-disulfonate dianion uses one $-SO_3$ unit to bind to two Sr^{II} cations and the other $-SO_3$ unit to bind to three Sr^{II} cations; of the two coordinated water molecules, one is monodentate to one Sr^{II} cation, whereas the other bridges two Sr^{II} cations. The μ_5-bridging mode of the dianon and the μ_2-bridging mode of the water molecule generate a polymeric three-dimensional network which is consolidated by O—H···O hydrogen bonds. The Sr^{II} cation exists in an undefined eight-coordinate environment.

Related literature

For a review of metal arenesulfonates, see: Cai (2004). For a related strontium naphthalenedisulfonate, see: Cai *et al.* (2001).



Experimental

Crystal data

$[Sr(C_{10}H_6O_6S_2)(H_2O)_2]$
M_r = 409.92
Orthorhombic, $Pna2_1$
a = 13.064 (6) Å
b = 19.324 (9) Å
c = 5.1989 (17) Å
V = 1312.5 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 4.46 mm^{-1}
T = 293 K
0.18 × 0.12 × 0.12 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.501, T_{max} = 0.616
11845 measured reflections
2962 independent reflections
2646 reflections with $I > 2\sigma(I)$
R_{int} = 0.040

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.071
S = 1.04
2962 reflections
190 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.60 e Å^{-3}
$\Delta\rho_{min}$ = −0.51 e Å^{-3}
Absolute structure: Flack (1983), 1584 Friedel pairs
Flack parameter: −0.011 (6)

Table 1
Selected bond lengths (Å).

Sr1—O1	2.612 (2)	Sr1—O6^{iv}	2.540 (2)
Sr1—O2^{i}	2.494 (2)	Sr1—O1w	2.614 (2)
Sr1—O3^{ii}	2.595 (2)	Sr1—O2w	2.756 (3)
Sr1—O5^{iii}	2.549 (2)	Sr1—O2w^{v}	2.974 (3)

Symmetry codes: (i) $-x, -y+1, z-\frac{1}{2}$; (ii) $-x, -y+1, z+\frac{1}{2}$; (iii) $-x+\frac{1}{2}, y+\frac{1}{2}, z+\frac{1}{2}$; (iv) $-x+\frac{1}{2}, y+\frac{1}{2}, z-\frac{1}{2}$; (v) $x, y, z+1$.

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1w—H1w1···O4^{vi}	0.84	2.29	3.066 (4)	154
O1w—H1w2···O4^{vii}	0.84	2.27	2.904 (4)	132
O2w—H2w2···O4^{vii}	0.84	2.03	2.856 (3)	167

Symmetry codes: (vi) $-x+1, -y+1, z+\frac{1}{2}$; (vii) $-x+1, -y+1, z-\frac{1}{2}$.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalClear* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5381).

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supporting information

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Poly[μ_2-aqua-aqua-μ_5-naphthalene-2,7-disulfonato-strontium]

Shan Gao and Seik Weng Ng

S1. Comment

A review of metal arenesulfonates that are synthesized in aqueous medium explains the reasons for the ability of the ions to form stable metal-organic frameworks owing to multiple coordination modes of the sulfonate $–SO_3$ groups (Cai, 2004). Among the divalent metal derivatives, the strontium system has been less studied (Cai *et al.*, 2001). In the crystal structure of $Sr(H_2O)_2(C_{10}H_6O_6S_2)$, the $C_{10}H_6O_6S_2^{2-}$ dianion uses one $–SO_3$ unit to bind to two Sr^{II} atoms and the other $–SO_3$ unit to bind to three Sr^{II} atoms; of the two water molecules, one is monodentate to one Sr atom whereas the other bridge two Sr atoms (Scheme I, Fig. 1). The μ_5-bridging mode of the dianon and the μ_2-bridging mode of the water molecule generates a polymeric three-dimensional network; the network is consolidated by O–H···O hydrogen bonds (Table 1). The Sr atom exists in an undefined eight-coordinate environment.

S2. Experimental

Strontium nitrate (1 mmol) and sodium naphthalene-2,7-disulfonate (1 mmol) were dissolved in water (10 ml). The solution was filtered and set aside; colorless crystals were isolated from the filtrate after several days.

S3. Refinement

Hydrogen atoms were generated geometrically and were included in the riding model approximation [C—H 0.93 Å and O–H 0.84 Å, U 1.2 to 1.5U_{eq}(C,O)]. The 3 7 2 reflection was omitted owing to bad agreement.

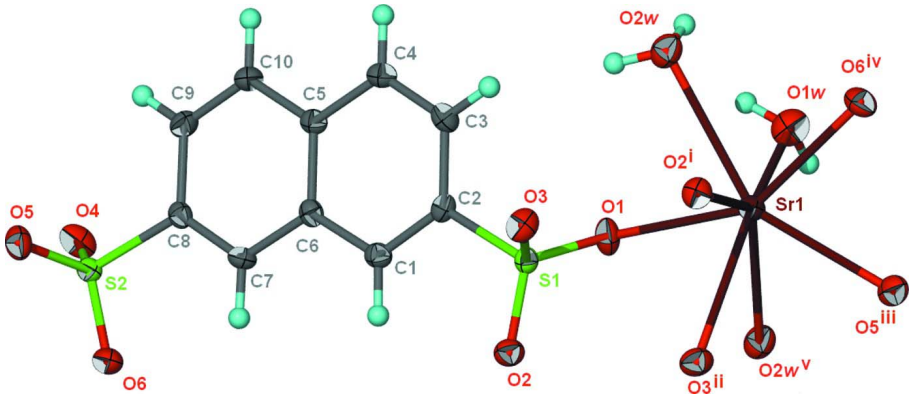

Figure 1

Thermal ellipsoid plot (Barbour, 2001) of a fragment of polymeric $Sr(H_2O)_2(C_{10}H_6O_6S_2)$ at the 50% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

Poly[μ_2-aqua-aqua-μ_5-naphthalene-2,7-disulfonato-strontium]

Crystal data

$[Sr(C_{10}H_6O_6S_2)(H_2O)_2]$
$M_r = 409.92$
Orthorhombic, $Pna2_1$
Hall symbol: P 2c -2n
$a = 13.064$ (6) Å
$b = 19.324$ (9) Å
$c = 5.1989$ (17) Å
$V = 1312.5$ (9) Å^3
$Z = 4$
$F(000) = 816$
$D_x = 2.075$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 10271 reflections
$\theta = 3.1$–$27.5°$
$\mu = 4.46$ mm^{-1}
$T = 293$ K
Prism, colorless
0.18 × 0.12 × 0.12 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scan
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.501$, $T_{max} = 0.616$
11845 measured reflections
2962 independent reflections
2646 reflections with $I > 2\sigma(I)$
$R_{int} = 0.040$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.1°$
$h = -16 \rightarrow 16$
$k = -24 \rightarrow 25$
$l = -6 \rightarrow 6$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.028$
$wR(F^2) = 0.071$
$S = 1.04$
2962 reflections
190 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0383P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.60$ e Å^{-3}
$\Delta\rho_{min} = -0.51$ e Å^{-3}
Absolute structure: Flack (1983), 1584 Friedel pairs
Absolute structure parameter: −0.011 (6)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Sr1	−0.008465 (18)	0.635847 (12)	0.49937 (9)	0.02043 (9)
S1	0.14037 (4)	0.47764 (3)	0.49983 (18)	0.01857 (14)
S2	0.64351 (5)	0.24848 (3)	0.49376 (18)	0.01863 (14)
O1	0.14590 (15)	0.55148 (11)	0.5589 (4)	0.0294 (6)
O2	0.12497 (16)	0.43544 (11)	0.7268 (4)	0.0256 (5)
O3	0.06622 (16)	0.46443 (12)	0.2980 (4)	0.0285 (5)
O4	0.74894 (15)	0.27350 (11)	0.5219 (6)	0.0310 (5)
O5	0.63559 (18)	0.19599 (11)	0.2968 (4)	0.0294 (5)
O6	0.59963 (17)	0.22808 (12)	0.7371 (4)	0.0288 (5)
O1w	0.13881 (15)	0.72744 (11)	0.5039 (7)	0.0376 (5)
H1w1	0.1543	0.7369	0.6567	0.056*
H1w2	0.1903	0.7113	0.4278	0.056*

O2w	0.08346 (17)	0.63163 (10)	0.0225 (6)	0.0315 (5)
H2w1	0.1187	0.5953	0.0242	0.038*
H2w2	0.1257	0.6644	0.0242	0.038*
C1	0.3192 (2)	0.40460 (13)	0.4846 (8)	0.0208 (5)
H1	0.2958	0.3826	0.6325	0.025*
C2	0.2615 (2)	0.45518 (15)	0.3713 (5)	0.0187 (6)
C3	0.2939 (2)	0.48863 (15)	0.1474 (6)	0.0240 (7)
H3	0.2526	0.5222	0.0717	0.029*
C4	0.3857 (2)	0.47221 (15)	0.0399 (6)	0.0230 (7)
H4	0.4072	0.4949	−0.1083	0.028*
C5	0.4485 (2)	0.42073 (15)	0.1525 (6)	0.0195 (6)
C6	0.4143 (2)	0.38578 (15)	0.3764 (6)	0.0196 (6)
C7	0.4773 (2)	0.33370 (14)	0.4836 (9)	0.0205 (6)
H7	0.4555	0.3097	0.6287	0.025*
C8	0.5694 (2)	0.31837 (15)	0.3767 (5)	0.0196 (6)
C9	0.6062 (3)	0.35484 (15)	0.1587 (6)	0.0247 (7)
H9	0.6707	0.3451	0.0920	0.030*
C10	0.5462 (2)	0.40419 (15)	0.0481 (6)	0.0241 (7)
H10	0.5694	0.4274	−0.0974	0.029*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sr1	0.02020 (14)	0.02060 (13)	0.02050 (13)	−0.00055 (9)	−0.00006 (17)	0.00153 (17)
S1	0.0168 (3)	0.0174 (3)	0.0215 (3)	0.0006 (2)	0.0002 (4)	−0.0011 (4)
S2	0.0182 (3)	0.0182 (3)	0.0195 (3)	−0.0003 (2)	−0.0002 (4)	0.0013 (4)
O1	0.0256 (12)	0.0186 (10)	0.0439 (18)	0.0013 (8)	0.0031 (10)	−0.0054 (9)
O2	0.0238 (12)	0.0276 (12)	0.0252 (11)	−0.0004 (9)	0.0028 (9)	0.0027 (9)
O3	0.0219 (12)	0.0363 (13)	0.0273 (11)	0.0012 (10)	−0.0039 (10)	−0.0047 (10)
O4	0.0206 (10)	0.0311 (11)	0.0414 (13)	−0.0040 (8)	−0.0073 (12)	0.0085 (14)
O5	0.0360 (14)	0.0235 (12)	0.0287 (12)	0.0056 (9)	−0.0051 (11)	−0.0047 (10)
O6	0.0355 (14)	0.0249 (11)	0.0260 (12)	0.0005 (10)	0.0050 (10)	0.0045 (10)
O1w	0.0341 (12)	0.0421 (13)	0.0366 (12)	−0.0059 (9)	−0.0008 (16)	−0.0050 (16)
O2w	0.0313 (11)	0.0307 (11)	0.0324 (13)	−0.0031 (9)	0.0037 (14)	−0.0060 (11)
C1	0.0234 (13)	0.0192 (12)	0.0197 (12)	−0.0033 (10)	−0.0004 (17)	−0.0003 (15)
C2	0.0143 (14)	0.0210 (14)	0.0210 (14)	−0.0008 (11)	−0.0003 (11)	−0.0046 (12)
C3	0.0243 (17)	0.0208 (14)	0.0270 (15)	0.0016 (12)	−0.0040 (14)	0.0028 (13)
C4	0.0253 (15)	0.0245 (14)	0.0193 (19)	−0.0021 (11)	−0.0002 (13)	0.0025 (12)
C5	0.0208 (16)	0.0184 (14)	0.0192 (15)	−0.0036 (12)	−0.0012 (12)	−0.0001 (12)
C6	0.0210 (16)	0.0159 (14)	0.0219 (14)	−0.0016 (12)	−0.0027 (12)	−0.0023 (12)
C7	0.0221 (13)	0.0210 (13)	0.0185 (14)	−0.0015 (10)	−0.0001 (16)	0.0049 (18)
C8	0.0224 (16)	0.0162 (14)	0.0202 (13)	0.0005 (12)	−0.0027 (12)	−0.0015 (11)
C9	0.0236 (17)	0.0257 (16)	0.0248 (16)	−0.0001 (12)	0.0064 (14)	0.0002 (13)
C10	0.0271 (16)	0.0243 (15)	0.021 (2)	0.0001 (12)	0.0041 (12)	0.0032 (12)

Geometric parameters (Å, º)

Sr1—O1	2.612 (2)	O1w—H1w2	0.8400
Sr1—O2^{i}	2.494 (2)	O2w—Sr1^{viii}	2.974 (3)
Sr1—O3^{ii}	2.595 (2)	O2w—H2w1	0.8400
Sr1—O5^{iii}	2.549 (2)	O2w—H2w2	0.8400
Sr1—O6^{iv}	2.540 (2)	C1—C2	1.367 (4)
Sr1—O1w	2.614 (2)	C1—C6	1.412 (4)
Sr1—O2w	2.756 (3)	C1—H1	0.9300
Sr1—O2w^{v}	2.974 (3)	C2—C3	1.397 (4)
S1—O2	1.448 (2)	C3—C4	1.360 (4)
S1—O3	1.451 (2)	C3—H3	0.9300
S1—O1	1.461 (2)	C4—C5	1.417 (4)
S1—C2	1.772 (3)	C4—H4	0.9300
S2—O6	1.444 (2)	C5—C6	1.418 (4)
S2—O5	1.445 (2)	C5—C10	1.423 (4)
S2—O4	1.467 (2)	C6—C7	1.414 (4)
S2—C8	1.769 (3)	C7—C8	1.358 (4)
O2—Sr1^{ii}	2.494 (2)	C7—H7	0.9300
O3—Sr1^{i}	2.595 (2)	C8—C9	1.418 (4)
O5—Sr1^{vi}	2.549 (2)	C9—C10	1.362 (4)
O6—Sr1^{vii}	2.540 (2)	C9—H9	0.9300
O1w—H1w1	0.8400	C10—H10	0.9300

O2^{i}—Sr1—O6^{iv}	78.25 (8)	S1—O3—Sr1^{i}	139.31 (13)
O2^{i}—Sr1—O5^{iii}	101.47 (8)	S2—O5—Sr1^{vi}	142.79 (14)
O6^{iv}—Sr1—O5^{iii}	72.56 (8)	S2—O6—Sr1^{vii}	147.99 (15)
O2^{i}—Sr1—O3^{ii}	75.53 (8)	Sr1—O1w—H1w1	109.5
O6^{iv}—Sr1—O3^{ii}	135.12 (7)	Sr1—O1w—H1w2	109.5
O5^{iii}—Sr1—O3^{ii}	77.77 (8)	H1w1—O1w—H1w2	109.5
O2^{i}—Sr1—O1	101.17 (7)	Sr1—O2w—Sr1^{viii}	130.23 (8)
O6^{iv}—Sr1—O1	149.72 (7)	Sr1—O2w—H2w1	104.7
O5^{iii}—Sr1—O1	135.70 (8)	Sr1^{viii}—O2w—H2w1	104.7
O3^{ii}—Sr1—O1	71.79 (7)	Sr1—O2w—H2w2	104.7
O2^{i}—Sr1—O1w	145.90 (10)	Sr1^{viii}—O2w—H2w2	104.7
O6^{iv}—Sr1—O1w	82.82 (8)	H2w1—O2w—H2w2	105.7
O5^{iii}—Sr1—O1w	99.51 (9)	C2—C1—C6	119.8 (3)
O3^{ii}—Sr1—O1w	135.57 (9)	C2—C1—H1	120.1
O1—Sr1—O1w	81.56 (8)	C6—C1—H1	120.1
O2^{i}—Sr1—O2w	74.84 (7)	C1—C2—C3	121.5 (3)
O6^{iv}—Sr1—O2w	75.06 (7)	C1—C2—S1	120.3 (2)
O5^{iii}—Sr1—O2w	147.45 (7)	C3—C2—S1	118.1 (2)
O3^{ii}—Sr1—O2w	130.00 (7)	C4—C3—C2	120.1 (3)
O1—Sr1—O2w	75.62 (7)	C4—C3—H3	120.0
O1w—Sr1—O2w	72.99 (10)	C2—C3—H3	120.0
O2^{i}—Sr1—O2w^{v}	138.66 (7)	C3—C4—C5	120.3 (3)
O6^{iv}—Sr1—O2w^{v}	134.37 (7)	C3—C4—H4	119.8
O5^{iii}—Sr1—O2w^{v}	73.79 (7)	C5—C4—H4	119.8

O3^{ii}—Sr1—O2w^{v}	63.25 (7)	C4—C5—C6	119.4 (3)
O1—Sr1—O2w^{v}	64.07 (7)	C4—C5—C10	121.3 (3)
O1w—Sr1—O2w^{v}	73.33 (9)	C6—C5—C10	119.2 (3)
O2w—Sr1—O2w^{v}	130.23 (8)	C1—C6—C7	122.6 (3)
O2—S1—O3	113.41 (13)	C1—C6—C5	118.8 (3)
O2—S1—O1	112.68 (14)	C7—C6—C5	118.6 (3)
O3—S1—O1	110.90 (13)	C8—C7—C6	120.6 (3)
O2—S1—C2	107.06 (13)	C8—C7—H7	119.7
O3—S1—C2	106.29 (14)	C6—C7—H7	119.7
O1—S1—C2	105.92 (13)	C7—C8—C9	121.2 (3)
O6—S2—O5	113.63 (13)	C7—C8—S2	120.7 (2)
O6—S2—O4	112.04 (16)	C9—C8—S2	118.0 (2)
O5—S2—O4	111.67 (15)	C10—C9—C8	119.4 (3)
O6—S2—C8	107.02 (14)	C10—C9—H9	120.3
O5—S2—C8	104.65 (14)	C8—C9—H9	120.3
O4—S2—C8	107.23 (14)	C9—C10—C5	120.8 (3)
S1—O1—Sr1	123.13 (12)	C9—C10—H10	119.6
S1—O2—Sr1^{ii}	149.15 (13)	C5—C10—H10	119.6

O2—S1—O1—Sr1	−99.69 (16)	O2—S1—C2—C1	1.7 (3)
O3—S1—O1—Sr1	28.67 (19)	O3—S1—C2—C1	−119.8 (3)
C2—S1—O1—Sr1	143.58 (13)	O1—S1—C2—C1	122.2 (3)
O2^{i}—Sr1—O1—S1	−14.73 (16)	Sr1—S1—C2—C1	151.7 (2)
O6^{iv}—Sr1—O1—S1	−100.53 (18)	O2—S1—C2—C3	179.3 (2)
O5^{iii}—Sr1—O1—S1	104.78 (16)	O3—S1—C2—C3	57.8 (2)
O3^{ii}—Sr1—O1—S1	55.81 (15)	O1—S1—C2—C3	−60.2 (3)
O1w—Sr1—O1—S1	−160.21 (17)	Sr1—S1—C2—C3	−30.7 (3)
O2w—Sr1—O1—S1	−85.71 (15)	C1—C2—C3—C4	−1.4 (4)
O2w^{v}—Sr1—O1—S1	124.29 (16)	S1—C2—C3—C4	−179.0 (2)
O3—S1—O2—Sr1^{ii}	−22.5 (3)	C2—C3—C4—C5	0.6 (4)
O1—S1—O2—Sr1^{ii}	104.6 (3)	C3—C4—C5—C6	0.9 (4)
C2—S1—O2—Sr1^{ii}	−139.4 (2)	C3—C4—C5—C10	−178.0 (3)
Sr1—S1—O2—Sr1^{ii}	64.1 (3)	C2—C1—C6—C7	−179.7 (3)
O2—S1—O3—Sr1^{i}	−62.7 (2)	C2—C1—C6—C5	0.7 (4)
O1—S1—O3—Sr1^{i}	169.39 (18)	C4—C5—C6—C1	−1.5 (4)
C2—S1—O3—Sr1^{i}	54.7 (2)	C10—C5—C6—C1	177.4 (3)
Sr1—S1—O3—Sr1^{i}	−173.4 (2)	C4—C5—C6—C7	178.9 (3)
O6—S2—O5—Sr1^{vi}	72.0 (3)	C10—C5—C6—C7	−2.2 (4)
O4—S2—O5—Sr1^{vi}	−160.0 (2)	C1—C6—C7—C8	−178.4 (3)
C8—S2—O5—Sr1^{vi}	−44.4 (3)	C5—C6—C7—C8	1.1 (5)
O5—S2—O6—Sr1^{vii}	0.2 (3)	C6—C7—C8—C9	1.4 (5)
O4—S2—O6—Sr1^{vii}	−127.6 (2)	C6—C7—C8—S2	−174.7 (2)
C8—S2—O6—Sr1^{vii}	115.2 (3)	O6—S2—C8—C7	−13.3 (3)
O2^{i}—Sr1—O2w—Sr1^{viii}	37.85 (9)	O5—S2—C8—C7	107.5 (3)
O6^{iv}—Sr1—O2w—Sr1^{viii}	−43.75 (10)	O4—S2—C8—C7	−133.7 (3)
O5^{iii}—Sr1—O2w—Sr1^{viii}	−49.76 (17)	O6—S2—C8—C9	170.5 (2)
O3^{ii}—Sr1—O2w—Sr1^{viii}	93.43 (12)	O5—S2—C8—C9	−68.6 (3)
O1—Sr1—O2w—Sr1^{viii}	143.91 (11)	O4—S2—C8—C9	50.1 (3)

O1w—Sr1—O2w—Sr1^{viii}	−130.67 (11)	C7—C8—C9—C10	−2.7 (5)
O2w^{v}—Sr1—O2w—Sr1^{viii}	180.0	S2—C8—C9—C10	173.4 (2)
S1—Sr1—O2w—Sr1^{viii}	123.51 (9)	C8—C9—C10—C5	1.6 (5)
C6—C1—C2—C3	0.7 (4)	C4—C5—C10—C9	179.7 (3)
C6—C1—C2—S1	178.3 (2)	C6—C5—C10—C9	0.8 (4)

Symmetry codes: (i) −*x*, −*y*+1, *z*−1/2; (ii) −*x*, −*y*+1, *z*+1/2; (iii) −*x*+1/2, *y*+1/2, *z*+1/2; (iv) −*x*+1/2, *y*+1/2, *z*−1/2; (v) *x*, *y*, *z*+1; (vi) −*x*+1/2, *y*−1/2, *z*−1/2; (vii) −*x*+1/2, *y*−1/2, *z*+1/2; (viii) *x*, *y*, *z*−1.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*w*—H1*w*1···O4^{ix}	0.84	2.29	3.066 (4)	154
O1*w*—H1*w*2···O4^{x}	0.84	2.27	2.904 (4)	132
O2*w*—H2*w*2···O4^{x}	0.84	2.03	2.856 (3)	167

Symmetry codes: (ix) −*x*+1, −*y*+1, *z*+1/2; (x) −*x*+1, −*y*+1, *z*−1/2.